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Padova
ITALY

Unconstrained Monotonic Calibration of Predictions in Deep Ranking Systems

USTC & Kuaishou Technology

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Outline

- Background
- Methodology
- Experiment
- Conclusion

Background

➢ What is Calibration

- **Ranking system** learns matching scores for sorting candidates

User Item

Recommendation

Query Document

Search

➡ Main focus: **relative order**

Larger score, larger similarity

- Accurate **absolute values** are essential for certain downstream tasks

Advertisement bidding

Expected Revenue (ER) = predicted Click-Through Rate (pCTR) × price

Assume price=10000, pCTR=0.8 → ER=8000
pCTR=0.9 → ER=9000

ΔpCTR=0.1 leads to ΔER=1000 !!!

Background

➢ How to Do Calibration

- Learn a **calibrator model** for adjustment

$$(\boldsymbol{x}, y, s)$$

Feature	Label	Score
User, Item, …	Binary 0/1, is_click	Prob. [0,1], pCTR

$$P(y=1|\boldsymbol{x}) \leftarrow s' = g_{\phi}(s, \boldsymbol{x}; \mathcal{D}),$$

Actual Prob. unobservable

Calibrated Prediction

Calibrator

- Calibration metrics for evaluation
  - We need the estimation of ground-truth P(y=1|x)

Aggregate samples with the same ____

- Score range (pCTR $\in [0.2, 0.4]$)
- Feature value (gender==man)

Expected Calibration Error (ECE)

Field Relative Calibration Error (FRCE)

Multi-Field Relative Calibration Error (MFRCE)

$$\mathrm{ECE} = \frac{1}{|\mathcal{D}|}\sum_{k=1}^{M}\Big|\sum_{(\boldsymbol{x},y,s)\in\mathcal{D}}(s'-y)\cdot\mathbb{I}\big(s'\in[\tfrac{k-1}{M},\tfrac{k}{M})\big)\Big|,$$

$$\mathrm{FRCE} = \frac{1}{|\mathcal{D}|}\sum_{k}\frac{|\sum_{(\boldsymbol{x},y,s)\in\mathcal{D}}(s'-y)\cdot\mathbb{I}(z=z_k)|}{|\sum_{(\boldsymbol{x},y,s)\in\mathcal{D}}y\cdot\mathbb{I}(z=z_k)|},$$

$$\mathrm{MFRCE} = \frac{1}{N_z}\sum_{z}\mathrm{FRCE},$$

Background

➢ Existing Work on Calibration

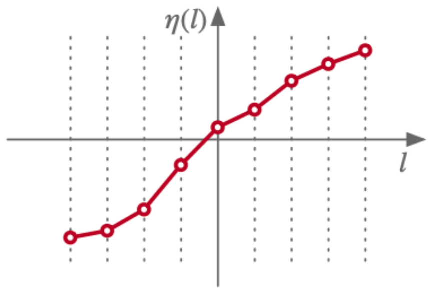
- Common process: $s \in [0,1] \xrightarrow{\sigma^{-1}} l \in (-\infty, +\infty) \rightarrow l' \in (-\infty, +\infty) \xrightarrow{\sigma^{-1}} s' \in [0,1]$

  Key: calibrate

  Original score — Original logit — New logit — New score

- Fixed-form **order-preserving** transformation
- **Simple transformation**
  - Platt scaling: learn a logistic regression function $l' = \dfrac{1}{1 + e^{-(al+b)}}$
  - Binning: Split samples into different bins based on l; $l' = \text{Binning}(l)$

    Statistically decide linear coefficients for each bins
  - **Limited parameter space**



Isotonic Line-Plot Scaling

Background

➢ Existing Work on Calibration

- **DNN-based transformation**
  - FAC (WWW'20): add DNN bias $l' = \text{Binning}(l) + \text{DNN}(\boldsymbol{x})$
  - SBCR (KDD'24): learn DNN-based linear coefficients $l' = \text{Binning}_{\text{DNN}}(l, \boldsymbol{x})$
  - DESC (KDD'24): learn DNN-based weights of basis functions $l' = w_{\text{DNN}}(\boldsymbol{x}) \cdot \boldsymbol{\mathcal{B}}(l)$

$$\mathcal{B}_i^{power}(t; h_i) = x^{h_i}$$

$$\mathcal{B}_i^{log}(t; v_i) = \frac{log(1 + v_i \cdot t)}{log(1 + v_i)}$$

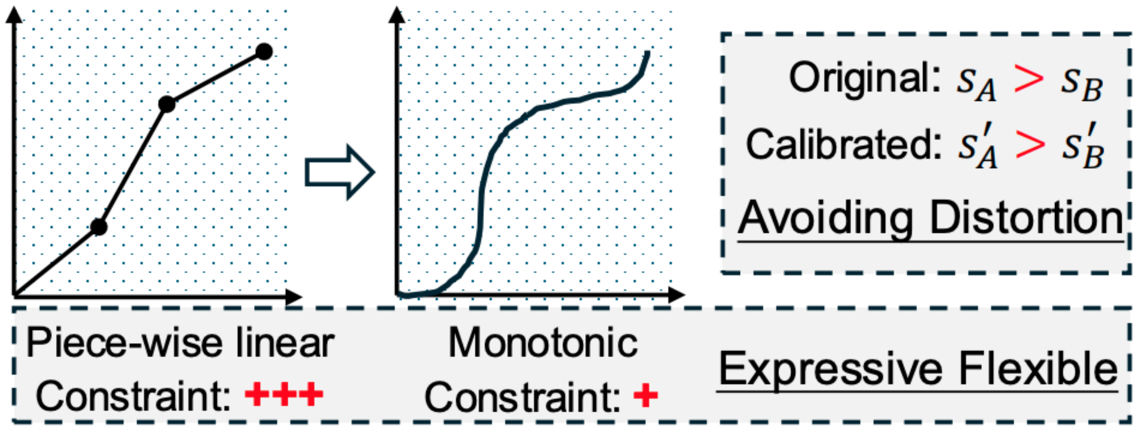
$$\mathcal{B}_i^{scaling}(t; a_i) = \sigma(\sigma^{-1}(t) \cdot a_i) \ ,$$

- **Limitation**
  - Excessive constraints: Most adhere to piece-wise linear
    - Fail in complex scenarios like <u>multi-field calibration</u>
    - Amplify value errors in specific fields within <u>feedback loops</u>
- **Motivation**: **reduce constraints** on the architecture for full potential

Methodology

➢ How to Reduce Constraints

- **Core idea**
  - Piece-wise linear = linear + monotonic
  - A more general form: **only monotonic**



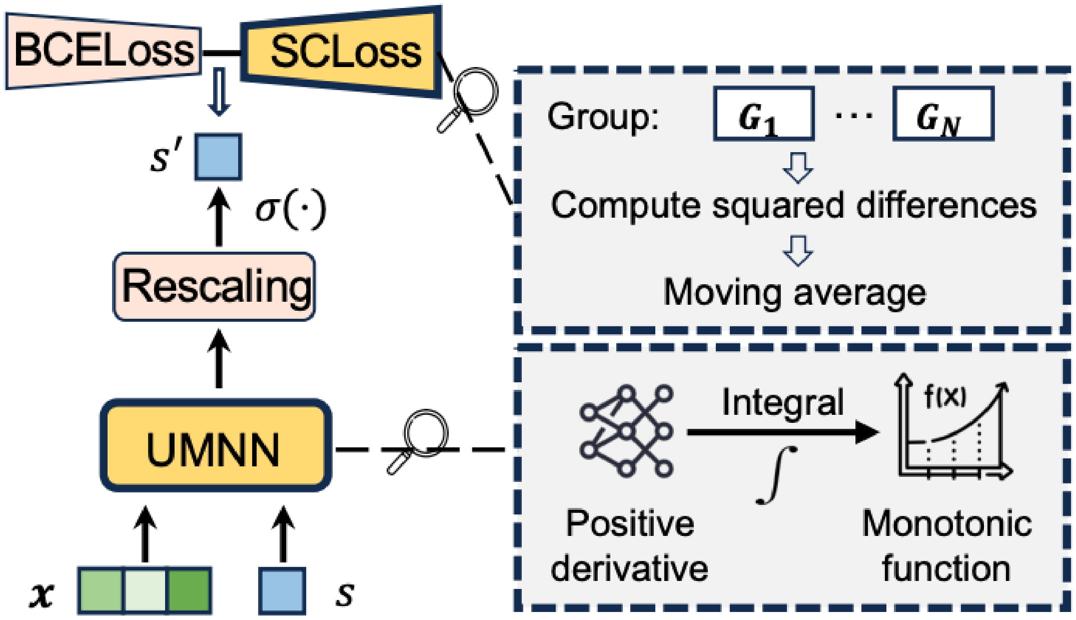
- How to design monotonicity
  - **UMNN** [1] is the answer
  - **Key**: if a function is differentiable, its derivative being single-sign is a necessary and sufficient condition for the function to be monotonic
  - **How**: construct a single-sign function and do integral computation

[1] Unconstrained Monotonic Neural Networks. NeurIPS 2019.

Methodology

➢ Overall Framework

- **Monotonic Calibrator Architecture**
  - UMNN to ensure monotonicity
  - Rescaling based on features
- **Calibration-aware Learning Strategy**
  - BCELoss
    - Common setting in previous work
  - SCLoss (Smooth Calibration Loss)
    - Specifically designed to emphasize calibration aspect



Methodology

➢ Monotonic Calibrator Architecture

☐ UMNN

- ☐ MLP with positive outputs $h(t,x) = 1 + \mathrm{ELU}(\mathrm{MLP}([t;x])),$
- ☐ Compute integral based on specific algorithm

Original logit

$$U(s,x) = \int_{t=0}^{\boxed{t=\sigma^{-1}(s)}} h(t,x)dt + \beta.$$

- ☐ Monotonicity is ensured by $\frac{d}{ds}U(s,x) = h(\sigma^{-1}(s),x)\cdot(\sigma^{-1}(s))' > 0,$

☐ Rescaling

- ☐ Features x are fed into a distinct MLP module $g_\phi(s,x) = \sigma(e^{w(x)}\cdot U(s,x) + b(x)).$
  - ☐ Compute a feature-specific rescaling factor $w(x)$ and bias term $b(x)$
  - ☐ Enhance the overall network learnability and preserve monotonicity
  - ☐ Apply Sigmoid to transform logit to score

Methodology

➢ Calibration-aware Learning Strategy

- **SCLoss**
  - Computation
    - Discretize the interval into N equal-width bins
    - Group samples by bins calibrated predictions fall into
    - Compute the squared differences per bin
    - Take a weighted average based on the group size
  - Moving average technique
    - Smooth by keeping a fraction of values from the previous batch

$$\mathrm{SCLoss}(\mathcal{B}) = \frac{1}{|\mathcal{B}|}\sum_{k=1}^{N} |G_k|(\bar{y}_k - \bar{s}'_k)^2,$$

$$G_k = \{(\boldsymbol{x}, y, s) \in \mathcal{B} \mid \frac{k-1}{N} \leq s' < \frac{k}{N}\},$$

$$\bar{y}_k \leftarrow \tau \cdot \bar{y}_k + (1-\tau) \cdot \frac{1}{|G_k|} \sum_{(\boldsymbol{x},y,s)\in G_k} y,$$

$$\bar{s}'_k \leftarrow \tau \cdot \bar{s}'_k + (1-\tau) \cdot \frac{1}{|G_k|} \sum_{(\boldsymbol{x},y,s)\in G_k} s',$$

- **Overall Loss** $\mathcal{L}(\mathcal{B}) = \mathrm{BCELoss}(\mathcal{B}) + \lambda \cdot \mathrm{SCLoss}(\mathcal{B}),$

Experiment

➢ Offline Experiment Setting

- **Dataset**
  - CTR dataset**:** Avazu, AliCCP
- **Evaluation**
  - Ranking: AUC, GAUC
  - Calibration (main focus): ECE, FRCE, MFRCE
- **Baseline**
  - Simple: Uncalib, HistBin, IsoReg, SIR, Platt, Gauss
  - DNN-based: FAC, SBCR, DESC
- **Pipline**
  - Train a DeepFM model, then train a calibrator model to calibrate predictions

Experiment

➢ Offline Experiment Result

Method	Avazu					AliCCP				
	AUC↑	GAUC↑	ECE↓	FRCE↓	MFRCE↓	AUC↑	GAUC↑	ECE↓	FRCE↓	MFRCE↓
Uncalib	0.7413	0.6544	0.0413	0.4207	0.3484	0.6348	0.5782	0.0202	1.4824	0.7291
HistBin [41]	0.7309	0.6368	0.0090	0.2701	0.2035	0.5239	0.5068	0.0076	1.2112	0.3909
IsoReg [42]	0.7413	0.6544	0.0088	0.2313	0.1655	0.6348	0.5782	0.0078	1.0168	0.3555
SIR [13]	0.7413	0.6544	0.0083	0.2147	0.1478	0.6348	0.5782	0.0080	1.0751	0.3721
Platt [33]	0.7413	0.6544	0.0109	0.2294	0.1606	0.6348	0.5782	0.0078	1.0179	0.3560
Gauss [26]	0.7413	0.6544	0.0095	0.2346	0.1640	0.6348	0.5782	0.0078	1.0180	0.3561
FAC [30]	0.7515	0.6649	0.0042	0.1473	0.0974	0.6358	0.5791	0.0065	0.9758	0.3186
SBCR [44]	0.7516	0.6651	0.0051	0.1416	0.0994	0.6362	0.5797	0.0063	0.9536	0.3096
DESC [40]	0.7514	0.6637	0.0074	0.1549	0.1086	0.6364	**0.5802**	0.0067	0.9697	0.3200
UMC (ours)	**0.7521**	**0.6654**	**0.0033**	**0.1172**	**0.0837**	**0.6367**	0.5801	**0.0058**	**0.9422**	**0.2951**

1. **Calib > Uncalib**: calibration is necessary for ranking models
2. **DNN-based > Simple**: enhanced model capacity
3. **UMC > baselines**: expressive calibrator & calibration-aware learning

Experiment

➢ Ablation Experiment Result

Table 3: Results of the ablation study for UMC on Avazu.

Method	AUC↑	GAUC↑	ECE↓	FRCE↓	MFRCE↓
Full UMNN	0.7521	0.6654	0.0033	0.1172	0.0837
w/o Rescaling	0.7508	0.6630	0.0078	0.1558	0.1118
w/o Feature	0.7413	0.6544	0.0080	0.2119	0.1465
w/o UMNN	0.7413	0.6544	0.0095	0.2482	0.1792
Full SCLoss	0.7521	0.6654	0.0033	0.1172	0.0837
w/o Average	0.7508	0.6626	0.0084	0.1613	0.1248
w/o SCLoss	0.7519	0.6651	0.0072	0.1672	0.1154
w/ MSELoss	0.7521	0.6649	0.0061	0.1512	0.0982

- **UMC w/o Rescaling**. This variant removes the rescaling layer of the architecture and relies solely on the UMNN output.
- **UMC w/o Feature**. This variant eliminates the feature input of the UMNN, resulting in a univariate mapping function.
- **UMC w/o UMNN**. This variant replaces the UMNN with a piecewise linear model in FAC.
- **UMC w/o Average**. This variant sets decay rate τ to zero, removing the exponential moving average usage of SCLoss.
- **UMC w/o SCLoss**. This variant sets balancing wight λ to zero, completely disables the effect of SCLoss.
- **UMC w/ MSELoss**. This variant replaces SCLoss with MSELoss, aligning the calibrated output with the binary label.

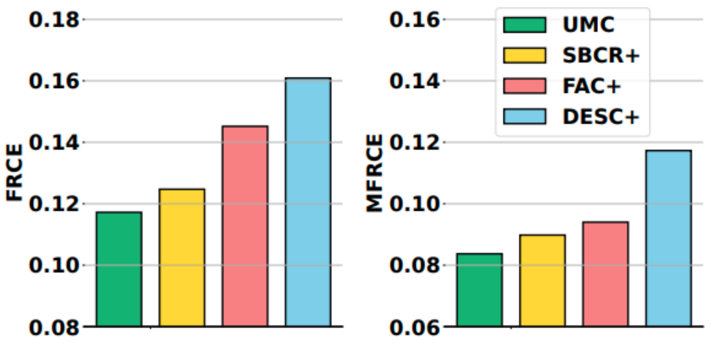


Figure 3: Results of adding SCLoss to other neural network-based baseline methods on Avazu.

1. Designs of UMNN and SCLoss are all effective
2. SCLoss can be generally applied to baselines

Experiment

➢ Hyper-parameter Experiment Result

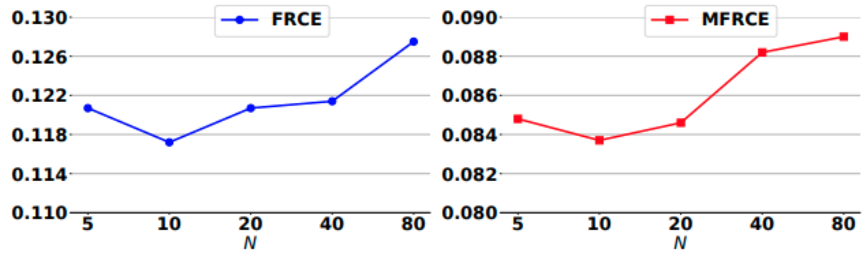


Figure 4: Results of the performance of UMC across different values of group number N on Avazu.

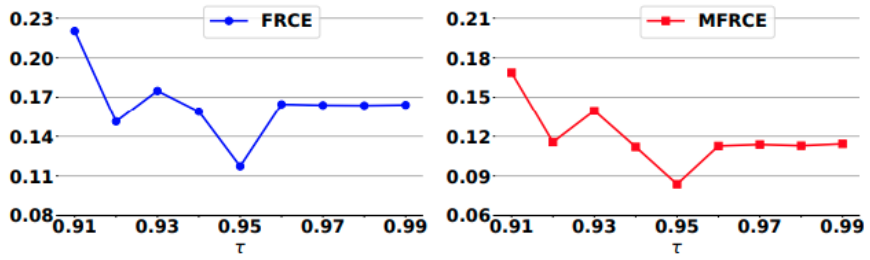


Figure 5: Results of the performance of UMC across different values of decay rate τ on Avazu.

$$\mathrm{SCLoss}(\mathcal{B}) = \frac{1}{|\mathcal{B}|}\sum_{k=1}^{N} |G_k|(\bar{y}_k - \bar{s}'_k)^2,$$

$$G_k = \{(\boldsymbol{x}, y, s) \in \mathcal{B} \mid \frac{k-1}{N} \le s' < \frac{k}{N}\},$$

Group number N in SCLoss

1. **Insufficient numbers** diminishes the ability to differentiate among groups
2. **Excessive numbers** can lead to bins with sparse data, rendering the computation unreliable

$$\bar{y}_k \leftarrow \tau \cdot \bar{y}_k + (1-\tau) \cdot \frac{1}{|G_k|} \sum_{(\boldsymbol{x},y,s) \in G_k} y,$$

$$\bar{s}'_k \leftarrow \tau \cdot \bar{s}'_k + (1-\tau) \cdot \frac{1}{|G_k|} \sum_{(\boldsymbol{x},y,s) \in G_k} s',$$

Decay rate τ in SCLoss

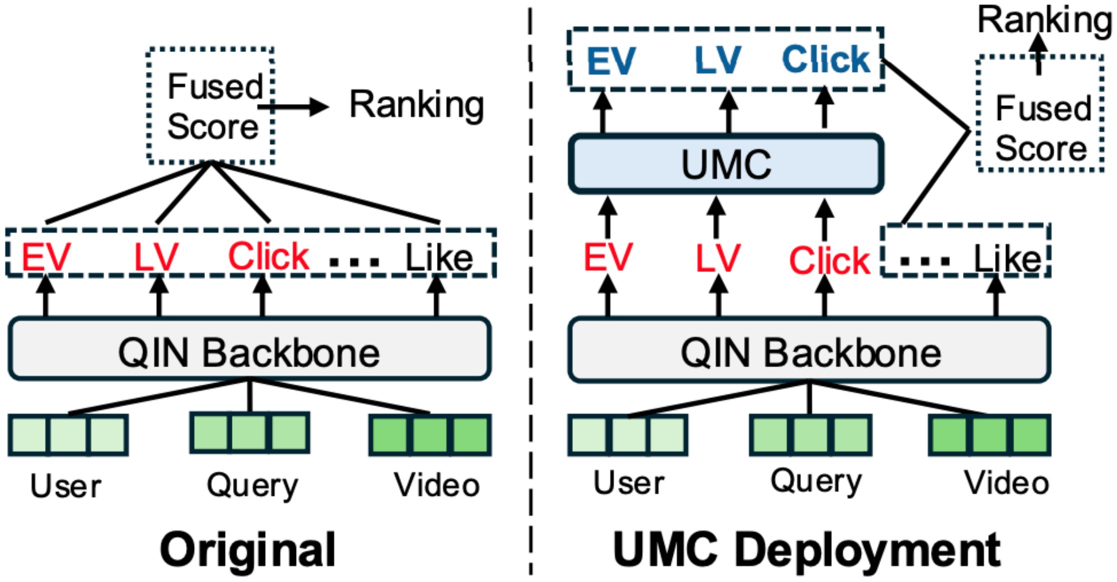
1. **Too small values** lead to a delayed response to recent batch data
2. **Too large value** obscure long-term trends

Experiment

➢ Online Experiment Result

◻ Kuaishou Video Search System

- ◻ Backbone: QIN [2]
- ◻ Scale: 5% (20 million users)
- ◻ Time: one week
- ◻ Method: **replace** the original predictions of **EffectiveView, LongView, Click** in the fused score



Metric	WT	VV	CTR
Improvement	**+0.414%**	**+0.411%**	**+0.170%**

- ◻ Metrics: total watch time (WT) effective video views (VV) and click-through rate (CTR)
- ◻ Note: **efficient** deployment without introducing significant computational overhead

[2] Query-dominant User Interest Network for Large-Scale Search Ranking. CIKM 2023.

Conclusion

- Calibration in Ranking System
  - **Challenge:** excessive calibrator constraints
  - **Motivation:** reduce constraints for a more general form
  - **Methodology**
    - Monotonic Calibrator Architecture (UMNN)
    - Calibration-aware Learning Strategy (SCLoss)
  - **Offline** experiment on real-world datasets
  - **Online** experiments on Kuaishou video search platform

Thanks

The code has been released at
https://github.com/baiyimeng/UMC